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Calculating critical orientations of polyhedra for similarity measure evaluation

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Abstract

This paper studies a problem related to the computation of similarity measures for two convex polyhedra based on Minkowski sums and mixed volumes. To compute the similarity measure a function has to be evaluated over a number so-called critical relative orientations of these polyhedra. An open problem in this area concerns the case that three edges of one polyhedron are parallel to three different faces of the other, and can be formulated as the question in how many ways a given triple of spherical points in the slope diagram representation of one polyhedron can be made to coincide with three edges of the slope diagram representation of the second polyhedron by rotation. Here we show that this number, which was so far only known to be finite, is in fact at most eight by reducing the problem to the solution of an 8th degree equation in one variable, which can be solved numerically.

Keywords

Similarity measure, Minkowski addition, slope diagram representation, spherical trigonometry, critical rotation.

I. INTRODUCTION

The notion of shape, and the similarity of shapes are important concepts in computer vision. In mathematical morphology these concepts are cast in well-defined mathematical notions and operations. In this field, recently a new family of methods has been developed [1] to calculate the similarity of two convex polyhedra. At the heart of these methods lies the Brunn-Minkowski inequality and its descendants, and the central operation is the calculation of Minkowski sums and mixed volumes. An attractive property of this family of similarity measures is that they are invariant under translations and possibly under scaling, rotation, and reflection. The method may be used in any-dimensional space, but we will concentrate on the 3D case.

To use this method for computing the similarity measure of two convex polyhedra, a function has to be evaluated over a number of relative orientations of these polyhedra. In [1] these relative orientations were defined in terms of so-called critical rotations, and it was shown that the number of such critical rotations is finite, but no more explicit upper bound could be given. In this paper a new method is derived to calculate all the required relative orientations in a finite number of steps. An upper bound for the maximum number of relative orientations is obtained as a by-product.

The goal of this paper is twofold. In the first place we want to sketch the essential concepts underlying this family of similarity measures. Therefore we will concentrate on one member of this family, the other ones being similar. This part is in an informal style. In the second part of this paper we switch to a more mathematical style, deriving expressions for the required relative orientations of the polyhedra.

II. PRINCIPLE OUTLINE

In this section the Minkowski sum, a Brunn-Minkowski like inequality, an instance of a similarity measure based on the Brunn-Minkowski like inequality, and the slope diagram representation of polyhedra are introduced.

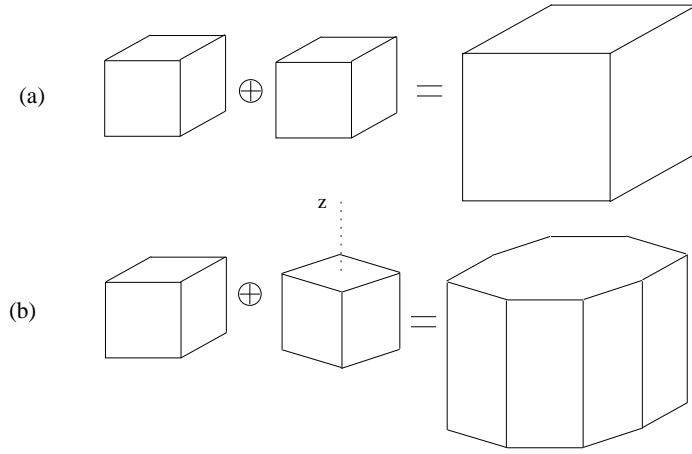


Fig. 1. Two cubes and their Minkowski sums. (a): the cubes have the same orientation. (b): one cube is rotated over $\frac{1}{4}\pi$ around the z-axis.

The Minkowski sum of two sets $A, B \subseteq \mathbb{R}^3$ is defined as

$$A \oplus B = \{a + b | a \in A, b \in B\}. \quad (1)$$

In Fig. 1 the Minkowski addition of two polyhedra is given for two different relative orientations, showing that the Minkowski sum depends on the relative orientations of the polyhedra. In Fig. 1(a) polyhedron B is identical to polyhedron A. In Fig. 1(b) polyhedron B is obtained by rotating polyhedron A over an angle $\frac{1}{4}\pi$ around the z-axis. Let $Vol(A)$ denote the volume of polyhedron A. After gaining some experience with Minkowski addition it is easily verified that in Fig. 1(a) the volumes of polyhedra $A \oplus B$, A and B are related by $Vol(A \oplus B) = 8Vol(A)^{\frac{1}{2}}Vol(B)^{\frac{1}{2}}$, and that (a bit more difficult) in Fig. 1(b) the inequality $Vol(A \oplus B) > 8Vol(A)^{\frac{1}{2}}Vol(B)^{\frac{1}{2}}$ holds. These facts are in accordance with the following theorem, derived from the Brunn-Minkowski inequality [1].

Theorem II.1: For two arbitrary polyhedra A and B in \mathbb{R}^3 ,

$$Vol(A \oplus B) \geq 8Vol(A)^{\frac{1}{2}}Vol(B)^{\frac{1}{2}} \quad (2)$$

with equality if and only if $A = B$.

Note that in (2) inequality holds when A and B are identical but have different spatial orientations. Using (2), a similarity measure σ may be constructed

$$\sigma(A, B) = \max_{R \in \mathcal{R}} \frac{8Vol(A)^{\frac{1}{2}}Vol(B)^{\frac{1}{2}}}{Vol(A \oplus R(B))} \quad (3)$$

where \mathcal{R} denotes the set of all spatial rotations, and where $R(B)$ denotes a rotation of B by R. Obviously, $0 \leq \sigma(A, B) \leq 1$, where $\sigma(A, B) = 1$ when $A = B$.

To find the maximum in (3), in principle orientations of B in all directions have to be checked. That would make (3) useless for practical purposes. Fortunately, as is shown in [1], to find the maximum value only a finite number of orientations of B has to be checked. Roughly speaking these orientations are characterized by the fact that planes and edges of B are as much as possible parallel to planes and edges of A. To formulate this more precisely we introduce the slope diagram representation (SDR) of polyhedra.

We will denote face i of polyhedron A by $F_i(A)$, edge j by $E_j(A)$, and vertex k by $V_k(A)$. The SDR of a polyhedron A, denoted by $SDR(A)$, is a unit sphere covered with spherical polygons. A vertex of A is represented by the interior of a polygon on $SDR(A)$, an edge by a spherical arc on $SDR(A)$, and a face by a vertex of some polygon on $SDR(A)$. To be more precise:

- *Face representation.* $F_i(A)$ is represented on the sphere by a point $SDR(F_i(A))$, located at the intersection of the outward unit normal vector u_i on $F_i(A)$ with the unit sphere.

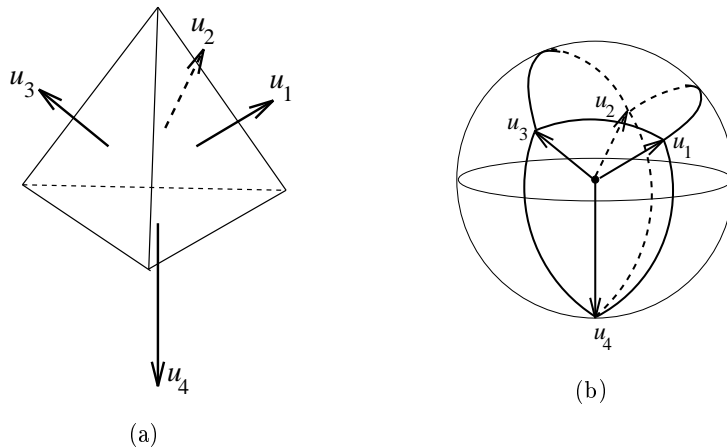


Fig. 2. Tetrahedron (a) and its slope diagram representation (b).

- *Edge representation.* An edge $E_j(A)$ is represented by the arc of the great circle connecting the two points corresponding to the two adjacent faces of $E_j(A)$.
- *Vertex representation.* A vertex $V_k(A)$ is represented by the interior of the polygon bounded by the arcs corresponding to the edges of A meeting at $V_k(A)$.

Note that $\text{SDR}(A)$ contains a complete description of A except its scale. In Fig. 2 an example of a polyhedron and its SDR is given.

Let us now see what it means in terms of $\text{SDR}(A)$ and $\text{SDR}(B)$ that faces and planes of B are parallel to faces and planes of A . It is easily verified that the faces $F_i(A)$ and $F_j(B)$ are parallel when $\text{SDR}(F_i(A))$ coincides with $\text{SDR}(F_j(B))$. Also, an edge $E_i(A)$ is parallel to $F_j(B)$ when $\text{SDR}(F_j(B))$ lies on $\text{SDR}(E_i(A))$.

As mentioned before, the maximum in (3) is obtained when the faces and edges of B are ‘as much as possible’ parallel to edges and faces of A . In [1] it is shown that only two situations have to be considered:

1. A face of B is parallel to a face of A and an edge of A is parallel to a face of B .
2. Three edges of A are parallel to three different faces of B .

To find the orientations of B described in the first case is trivial. When a face $F_j(B)$ is parallel to a face $F_i(A)$, B has only degree of freedom left, being a rotation around an axis through the origin and $\text{SDR}(F_j(B))$. Using the slope diagram representations of A and B , it is easy to find those rotations of B (finite in number [2]) around this axis that make the slope diagram representations of faces of B coincide with the slope diagram representations of edges of A .

To find the orientations of B described in the second case is more complex. It is asked to find those orientations of B where three points on $\text{SDR}(B)$ (representing three faces of B), lie on three spherical arcs on $\text{SDR}(A)$. In [1] it was shown that the number of such relative orientations is finite. The main contribution of this paper is to show that this number is at most eight. We were not able to find direct method for solving this problem for spherical *arcs*, but only for great circles containing these arcs. From these solutions, those ones can be selected with the points located on the arcs. In the remainder of the paper this method will be derived. It is shown that for every three points on $\text{SDR}(B)$ and every three great circles on $\text{SDR}(A)$ there are at most eight orientations of B such that the points are on the great circles.

III. CALCULATING CRITICAL ORIENTATIONS

Problem Formulation I: Given is a unit sphere with a spherical triangle with vertices a', b', c' and three great circles k', l', m' . Find the orthogonal transformation \mathbf{R}' that moves the triangle $a'b'c'$, in such a way that a' lies on k' , b' lies on l' , and c' lies on m' .

Problem Formulation II: In 3D space three vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are given and three fixed vectors $\mathbf{k}', \mathbf{l}', \mathbf{m}'$, with $|\mathbf{a}' \ \mathbf{b}' \ \mathbf{c}'| \neq 0$ and $|\mathbf{k}' \ \mathbf{l}' \ \mathbf{m}'| \neq 0$, where $|\mathbf{k} \ \mathbf{l} \ \mathbf{m}|$ is the determinant of the matrix with column vectors

$\mathbf{k}, \mathbf{l}, \mathbf{m}$. Find the proper orthogonal transformation \mathbf{R}' that moves the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$, such that

$$\mathbf{k}' \cdot (\mathbf{R}'\mathbf{a}') = 0, \quad \mathbf{l}' \cdot (\mathbf{R}'\mathbf{b}') = 0, \quad \mathbf{m}' \cdot (\mathbf{R}'\mathbf{c}') = 0, \quad (4)$$

where ‘proper’ is defined as $|\mathbf{R}'| = 1$. In words the problem is to find the rotation \mathbf{R}' that moves the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ such that \mathbf{a}', \mathbf{b}' resp. \mathbf{c}' are perpendicular to \mathbf{k}', \mathbf{l}' resp. \mathbf{m}' .

Problem formulations I and II are related as follows (Fig. 3). Let us assume that the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ have unit length. Then a' is the intersection of \mathbf{a}' with the sphere, and b' and c' are defined analogously. The great circles k', l' and m' result from the intersection of the sphere with the origin-crossing planes perpendicular to the vectors $\mathbf{k}', \mathbf{l}', \mathbf{m}'$.

A. Solution outline

Unless otherwise stated we will concentrate in the following on solving the problem as stated in formulation II. To arrive at a solution, three important choices are made:

1. We do not solve (4) for $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ at their original position, but precondition the problem by moving these two vector-triples to special relative and absolute positions.
2. In order to avoid the use of trigonometric functions, for the most crucial rotation we will use the Rodrigues formalism. Thanks to this formalism and due to the special positions of the two vector-triples, the problem boils down to solving two coupled polynomial equations in two variables.
3. To solve the two polynomial equations they are uncoupled, giving an 8th degree equation in one variable and an explicit expression for the other variable.
4. The 8th degree equation is solved numerically. Each real root corresponds to a solution of the original problem.

B. Repositioning $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ and $\mathbf{a}', \mathbf{b}', \mathbf{c}'$

We do not solve (4) for $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ at their original position. Instead, the triple $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ is transformed by an orthogonal transformation \mathbf{S}

$$\mathbf{k} = \mathbf{S}\mathbf{k}', \quad \mathbf{l} = \mathbf{S}\mathbf{l}', \quad \mathbf{m} = \mathbf{S}\mathbf{m}', \quad (5)$$

such that \mathbf{k} coincides with the z-axis, and \mathbf{l} lies in the y-z plane. Transforming the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ with \mathbf{S} gives

$$\mathbf{a}'' = \mathbf{S}\mathbf{a}' \quad \mathbf{b}'' = \mathbf{S}\mathbf{b}' \quad \mathbf{c}'' = \mathbf{S}\mathbf{c}'. \quad (6)$$

Now we move the vectors $\mathbf{a}'', \mathbf{b}''$ and \mathbf{c}'' by an orthogonal transformation \mathbf{T} ,

$$\mathbf{a} = \mathbf{T}\mathbf{a}'', \quad \mathbf{b} = \mathbf{T}\mathbf{b}'', \quad \mathbf{c} = \mathbf{T}\mathbf{c}'', \quad (7)$$

such that \mathbf{a} coincides with the x-axis and \mathbf{b} lies in the x-y plane.

Let us assume for the moment that in the unprimed situation we have found an orthogonal transformation \mathbf{R} , such that

$$\mathbf{k} \cdot \mathbf{R}\mathbf{a} = 0 \quad \mathbf{l} \cdot \mathbf{R}\mathbf{b} = 0 \quad \mathbf{m} \cdot \mathbf{R}\mathbf{c} = 0. \quad (8)$$

Moreover, let us assume that the transformations \mathbf{S} and \mathbf{T} are known. Then, using (5)–(8), equation (4) may be written as

$$\mathbf{k}' \cdot \mathbf{S}^{-1}\mathbf{R}\mathbf{T}\mathbf{S}\mathbf{a}' = 0 \quad \mathbf{l}' \cdot \mathbf{S}^{-1}\mathbf{R}\mathbf{T}\mathbf{S}\mathbf{b}' = 0 \quad \mathbf{m}' \cdot \mathbf{S}^{-1}\mathbf{R}\mathbf{T}\mathbf{S}\mathbf{c}' = 0. \quad (9)$$

This means that \mathbf{R}' , which is our ultimate goal, may be written as

$$\mathbf{R}' = \mathbf{S}^{-1}\mathbf{R}\mathbf{T}\mathbf{S}. \quad (10)$$

As we will show in a later section, finding the transformations \mathbf{S} and \mathbf{T} is trivial, so our main task will be to solve (8) for \mathbf{R} .

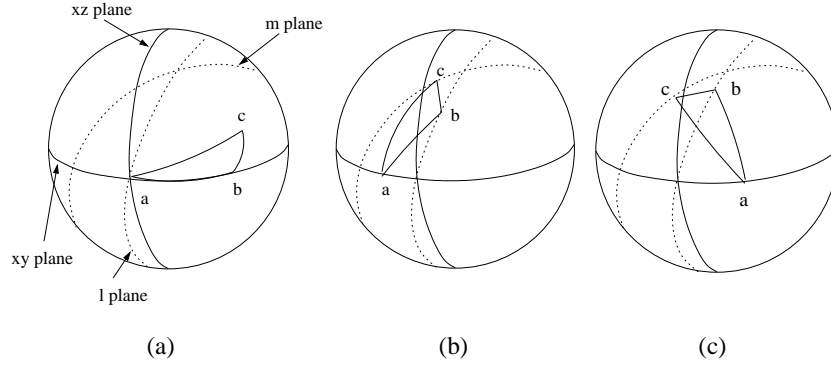


Fig. 3. (a): The situation after preconditioning the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{k}', \mathbf{l}', \mathbf{m}'$. The l plane and the m plane are the planes normal to the vectors \mathbf{l} and \mathbf{m} (not shown). The k plane coincides with the xy plane. (b): One of the solutions of (8). (c): Another solution of (8).

Let us finally give explicitly the vectors $\mathbf{k}, \mathbf{l}, \mathbf{m}$ and $\mathbf{a}, \mathbf{b}, \mathbf{c}$. As a result of the transformations in (5)–(7) they are

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ 0 \end{pmatrix}, \mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}, \mathbf{k} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \mathbf{l} = \begin{pmatrix} 0 \\ l_2 \\ l_3 \end{pmatrix}, \mathbf{m} = \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix} \quad (11)$$

In the following we assume without loss of generality that the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}', \mathbf{k}', \mathbf{l}', \mathbf{m}'$ and the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{k}, \mathbf{l}, \mathbf{m}$ have unit length.

C. The Rodrigues matrix

Every proper orthogonal transformation may be considered as a rotation over some angle around an axis. We will represent this rotation axis by

$$\mathbf{r} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}. \quad (12)$$

The length $r = \|\mathbf{r}\|$ of this vector is used to define the angle of rotation θ around this axis by

$$\tan\left(\frac{\theta}{2}\right) = r. \quad (13)$$

According to Rodrigues, see e.g. [3], this rotation may be represented by a matrix

$$\mathbf{R} = \left(\frac{1}{1 + u^2 + v^2 + w^2} \right) \begin{pmatrix} 1 + u^2 - v^2 - w^2 & 2(uv - w) & 2(uw + v) \\ 2(uv + w) & 1 - u^2 + v^2 - w^2 & 2(vw - u) \\ 2(uw - v) & 2(vw + u) & 1 - u^2 - v^2 + w^2 \end{pmatrix}. \quad (14)$$

So, a rotation of some vector \mathbf{d} around \mathbf{r} over an angle θ given by (13) may be written as

$$\mathbf{d}' = \mathbf{R}\mathbf{d}. \quad (15)$$

D. Deriving and solving the polynomial equations in u, v, w .

We are now ready to write down (8) explicitly. To this end, we will use the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{k}, \mathbf{l}, \mathbf{m}$ as given in (11). For \mathbf{R} we do not take the complete expression in (14) but only the matrix part, i.e. we leave out the factor $(1 + u^2 + v^2 + w^2)^{-1}$. This is allowed because, when it comes to two vectors being orthogonal, only the directions of these vectors matter, not their lengths. So, (8) may be expanded into the following three equations:

$$2(uw - v) = 0, \quad (16)$$

$$l_2(2b_1(uv + w) + b_2(1 - u^2 + v^2 - w^2)) + 2l_3b_2(vw + u) = 0, \quad (17)$$

$$\begin{aligned}
& m_1(c_1(1 + u^2 - v^2 - w^2) + 2c_2(uv - w) + 2c_3(uw + v)) + \\
& m_2(2c_1(uv + w) + c_2(1 - u^2 + v^2 - w^2) + 2c_3(vw - u)) + \\
& m_3(2c_2(vw + u) + c_3(1 - u^2 - v^2 + w^2)) = 0.
\end{aligned} \tag{18}$$

Using (16) to eliminate v from (17) and (18) gives two equations in u and w :

$$l_2(2b_1(u^2w + w) + b_2(1 - u^2 + u^2w^2 - w^2)) + 2l_3b_2(uw^2 + u) = 0, \tag{19}$$

and

$$\begin{aligned}
& m_1(c_1(1 + u^2 - u^2w^2 - w^2) + 2c_2(u^2w - w) + 4c_3(uw)) + \\
& m_2(2c_1(u^2w + w) + c_2(1 - u^2 + u^2w^2 - w^2) + 2c_3(uw^2 - u)) + \\
& m_3(2c_2(uw^2 + u) + c_3(1 - u^2 - u^2w^2 + w^2)) = 0.
\end{aligned} \tag{20}$$

We uncouple these two non-linear equations by using (19) to eliminate w from (20). By using the method of pseudo-resultants, the computer-algebra program MAPLE[©]¹ succeeds in this task, giving two expressions

$$f_0 + f_1u + f_2u^2 + f_3u^3 + f_4u^4 + f_5u^5 + f_6u^6 + f_7u^7 + f_8u^8 = 0, \tag{21}$$

$$w = w(u, b_1, b_2, c_1, c_2, c_3, l_2, l_3, m_1, m_2, m_3). \tag{22}$$

The first expression is an eighth degree equation in u , with real coefficients f_i , $0 \leq i \leq 8$, only depending on $b_1, b_2, c_1, c_2, c_3, l_2, l_3, m_1, m_2, m_3$. In the second expression, w is given explicitly as a polynomial function of u and $b_1, b_2, c_1, c_2, c_3, l_2, l_3, m_1, m_2, m_3$. We do not give (21) and (22) in full form, because, as is usual with this kind of results, the complete expressions are long, one page each, and do not give additional insight.

For given vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{k}, \mathbf{l}, \mathbf{m}$, (21) may be solved numerically. For this we use Laguerre's method [4]. Of the resulting values for u , the real ones are used in (22) to give w . Substituting the real values for u and w into (16) gives v . Subsequently, \mathbf{R} as given in (14) may be calculated, and finally \mathbf{R}' as given in (10).

E. Calculating \mathbf{S} and \mathbf{T}

Let us first deal with \mathbf{S} . The orthogonal preconditioning matrix \mathbf{S} , as introduced in (5), should rotate the vectors $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ such that \mathbf{k} coincides with the z axis, and \mathbf{l} lies in the y - z plane, i.e. $k_1 = 0, k_2 = 0, k_3 = 1, l_1 = 0$. With this specification the sign of l_2 remains free. We choose it to be positive.

Equation (5) suggests that we first find \mathbf{S} , and subsequently use it to calculate the vectors $\mathbf{k}, \mathbf{l}, \mathbf{m}$. However, it is more practical to first calculate $\mathbf{k}, \mathbf{l}, \mathbf{m}$ in some way, and then use these vectors to calculate \mathbf{S} . Knowing $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ and $\mathbf{k}, \mathbf{l}, \mathbf{m}$, and assuming that (5) holds, \mathbf{S} is given by

$$\mathbf{S} = (\mathbf{k} \ \mathbf{l} \ \mathbf{m})(\mathbf{k}' \ \mathbf{l}' \ \mathbf{m}')^{-1}, \tag{23}$$

where $(\mathbf{k} \ \mathbf{l} \ \mathbf{m})$ is the matrix with column vectors $\mathbf{k}, \mathbf{l}, \mathbf{m}$, and similarly for $(\mathbf{k}' \ \mathbf{l}' \ \mathbf{m}')$.

Constructing manually the vectors $\mathbf{k}, \mathbf{l}, \mathbf{m}$ for given $\mathbf{k}', \mathbf{l}', \mathbf{m}'$ goes as follows. Recall that the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}', \mathbf{k}', \mathbf{l}', \mathbf{m}'$ have unit length, and that the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{k}, \mathbf{l}, \mathbf{m}$ should have unit length. The vector \mathbf{k} is given in (11) already. The vector \mathbf{l} is given by

$$\mathbf{l} = \begin{pmatrix} 0 \\ (1 - \mathbf{k}' \cdot \mathbf{l}'^2)^{1/2} \\ \mathbf{k}' \cdot \mathbf{l}' \end{pmatrix}. \tag{24}$$

This is because the equality $\mathbf{k}' \cdot \mathbf{l}' = \mathbf{k} \cdot \mathbf{l}$ should hold, and because \mathbf{l} should have unit length.

To find \mathbf{m} , we first express \mathbf{m}' in terms of \mathbf{k}', \mathbf{l}' and $\mathbf{k}' \times \mathbf{l}'$. This may be done by solving $\alpha_1, \alpha_2, \alpha_3$ from

$$(\mathbf{k}' \ \mathbf{l}' \ \mathbf{k}' \times \mathbf{l}') \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \mathbf{m}'. \tag{25}$$

¹MAPLE is a trademark of Waterloo Maple inc.

Using $\alpha_1, \alpha_2, \alpha_3$, \mathbf{m} is given by

$$\mathbf{m} = \alpha_1 \mathbf{k} + \alpha_2 \mathbf{l} + \alpha_3 \mathbf{k} \times \mathbf{l}. \quad (26)$$

Herewith, the vectors $\mathbf{k}, \mathbf{l}, \mathbf{m}$ are known, so \mathbf{S} may be calculated with (23). The preconditioning matrix \mathbf{T} may be calculated analogously by using (6) and (7).

F. Implementation

We implemented the foregoing formulas in single precision and visualized the successive stages of the process. For purpose of comparison, and using only formulae from conventional spherical trigonometry, we also wrote a program that moves the vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ such that only the first two conditions of (4) are fulfilled, i.e. the triple $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ may move with one degree of freedom. In this way the vector \mathbf{c}' moves along a curve, and the value of $\mathbf{m}' \cdot \mathbf{c}'$ may be monitored. Those positions of \mathbf{c}' where $\mathbf{m}' \cdot \mathbf{c}' = 0$ are the solutions of (4). They were used to test the method we propose.

We compared the results of both methods for a number of cases. Both methods gave the same number of solutions, and the solutions were, within numerical precision, the same. As equation (21) indicates, the number of solution ranges from zero to eight. In the tests we did, the number of real solutions was always even, i.e. 0, 2, 4, 6 and 8. That we did not find an uneven number of solutions is because for that to happen, equation (21) should have multiple roots, which is a very unlikely situation in real numerical calculations. Note that complex solutions occur in pairs because the coefficients in (21) are real.

In order to test the accuracy of the method we calculated for every solution the value

$$\epsilon = |\mathbf{k}' \cdot (\mathbf{R}' \mathbf{a}')| + |\mathbf{l}' \cdot (\mathbf{R}' \mathbf{b}')| + |\mathbf{m}' \cdot (\mathbf{R}' \mathbf{c}')|. \quad (27)$$

In our implementation ϵ was on the average 10^{-8} with worst case values of 10^{-7} . By using a simple root polishing method the precision could always be improved to 10^{-9} .

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